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The formation of a high number density of helium bubbles in FCC metals irradiated within the fusion energy environment is well established. Yet, the role of helium bubbles in radiation hardening and mechanical property degradation of these steels remains an outstanding issue. In this paper, we present the results of a combined molecular dynamics simulation and in-situ straining transmission electron microscopy study, which investigates the interaction mechanisms between glissile dislocations and nanometer-sized helium bubbles. The molecular dynamics simulations, which directly account for dislocation core effects through semi-empirical interatomic potentials, provide fundamental insight into the effect of helium bubble size and internal gas pressure on the dislocation/bubble interaction and bypass mechanisms. The combination of simulation and in-situ straining experiments provides a powerful approach to determine the atomic to microscopic mechanisms of dislocation-helium bubble interactions, which govern the mechanical response of metals irradiated within the fusion environment.

INTRODUCTION

Predicting the in-service performance of metals in fusion energy facilities remains a major scientific challenge. Materials, especially those exposed to radiation or continued thermo-cycling have continually evolving microstructures which alter the corresponding physical and mechanical properties of the metal. It is well established that exposure to increasing irradiation dose generally leads to increased yield strength and decreased ductility [1-5]. While many of the basic sources of irradiation induced hardening are understood, predictive models of the mechanical property changes in irradiated materials do not exist. Atomistic insight into the bypass mechanisms of dislocations surmounting nanometer voids and helium bubbles is one key aspect of the additional knowledge of deformation mechanisms and their activation under

various irradiation conditions required as input to predictive models.

Computer simulations and in-situ transmission electron microscopy (TEM) are two powerful tools [2, 6] which allow examination of these questions at the atomic and nano-scale levels. This study examines the interactions between edge dislocations in FCC metals and nanometer-sized He bubbles over a range of internal gas pressures. The results not only provide insight to the deformation modes at an atomic level but also provide accurate estimates of key material parameters which are central to dispersed obstacle hardening models, dislocation dynamics simulations and constitutive models of material behavior.

PROCEDURE

Molecular dynamics (MD) simulations are an ideal tool to investigate deformation phenomena since they directly account for core and non-linear effects not treated within elastic theory. The motion of edge dislocations and their interactions with obstacles in aluminum have been studied using the molecular dynamics code MDCASK [7]. The simulation system has basis vectors along the $X = [\bar{1}11]$, $Y = [110]$ and $Z = [1\bar{1}2]$ directions and is 50x100x60 lattice units in size. Periodic boundary conditions are used in the Y and Z directions while the $X = [\bar{1}11]$ faces are traction-controlled, but otherwise free surfaces. Each system contains approximately two million atoms. The Ercolessi and Adams force-matching embedded atom method potential [8] is used to model the Al/Al interactions while pair potentials are used for the Al/He interactions and He/He interactions.

An edge dislocation is introduced into the cell by removing two (220) half planes. Helium bubbles are introduced by removing a 2.6 nm diameter sphere of atoms and introducing the desired number of helium atoms. The geometry is such that the glide plane of the dislocation runs along the diameter of the bubble. Helium/lattice site ratios of 0.0 (i.e., a void), 0.5, 1.0 and 2.0 are considered. Dislocation motion is then studied as a function of applied shear stress by applying a constant surface traction in the [110] direction to the atoms in the two $(\bar{1}11)$ surfaces.

In-situ TEM is one of the few experimental tools capable of directly observing the interactions between dislocations and obstacles [2, 6]. Thin foils of Cu were irradiated at 500ºC with 30keV He+ ions to a dose of 6.76×10^{15} ions cm^{-2}. Straining of the irradiated specimens was performed at room temperature on a JEOL 4000EX TEM at 300kV. A Gatan TV-rate camera is used to record the dynamic events.

RESULTS/DISCUSSION

The pressure required to balance the surface tension of a spherical cavity is given by

$$P_{equil} = \frac{2.0\gamma}{r}$$

For 2.6nm bubbles in aluminum this results in an equilibrium pressure of 1500 MPa. Simulations were conducted to examine the effect of bubble pressure on the local FCC crystal structure and the interaction with dislocations. While under pressurized bubbles, defined as having He/lattice ratios of 1 or less ($P < P_{equil}$), do not disturb the FCC lattice; over pressurized ($P > P_{equil}$) helium bubbles, such as He/lattice=2 (5800 MPa), lead to severe disruption of the nearby FCC lattice, including the production of self - interstitial clusters [9], as shown in Figure 1. Helium bubble pressures were estimated using the Mills, Liebenber and Bronson equation of state [10].

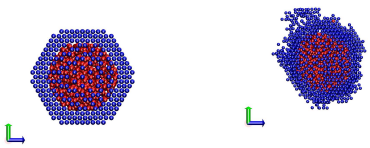

Figure 1. Under pressurized bubbles (left) do not disrupt the FCC lattice. Over pressurized bubbles cause 'punching'. The red atoms are helium atoms and blue are aluminum.

The interaction between a periodic array of moving edge dislocations as well as the eventual fate of the bubbles has been examined. The bypass mechanism in systems containing under pressurized bubbles involves the shearing of the bubble by one Burgers vector with each passage of the dislocation. At the atomic scale, the dislocation segment locally annihilates at the leading surface of the bubble and re-nucleates on the trailing surface as it breaks away from the obstacle. In these simulations, no evidence of impenetrable obstacles was observed, e.g., Orowan looping did not occur.

Characterization of the obstacle strength is key to predicting the properties of irradiated materials. Unfortunately, high strain rate molecular dynamics simulations underestimate the critical angle thus leading to an over estimate of the obstacle hardness.

To more accurately determine the strength of the bubble, a series of simulations have been preformed in which the applied shear stress is decreased from 100 MPa to a critical stress at which the dislocation is just able to shear the bubble. While the critical applied shear stress for a void is less than 25 MPa, that of an under-pressurized bubble with He/lattice ratio = 0.5 (i.e., 90 MPa) bubble is determined to be approximately 35 MPa. Further simulations will continue to quantify the effect of He pressure on

the critical stress, as well as to quantify the effect of image interactions from the periodic array of dislocations/obstacles.

Analysis of in-situ TEM straining of He implanted copper specimens provides information about both the dynamic interactions of dislocations with He bubbles to compare with the MD simulations and a quantitative analysis of the critical shear stress required for breakaway. Examination of the bubbles formed during the He implantation reveals a mean bubble size of 6 nm, and an estimated bubble pressure of 60 MPa. As the simulations demonstrated, the dislocation interacts with the free surface of the bubbles and it is the detachment of the dislocation from the bubble that is the controlling process. Figure 2 shows the experimental distribution of critical shear stresses as determined from a line tension balance relation calculated at breakaway. While the average critical stress is 113 MPa a large distribution of stresses is observed, emphasizing the importance of the local interaction geometry on the resulting obstacle strength. The experimental results are in reasonable agreement with the MD simulations, recalling that the product of the shear modulus and the Burgers vector (Gb), is approximately 2.5 larger in copper than in aluminum.

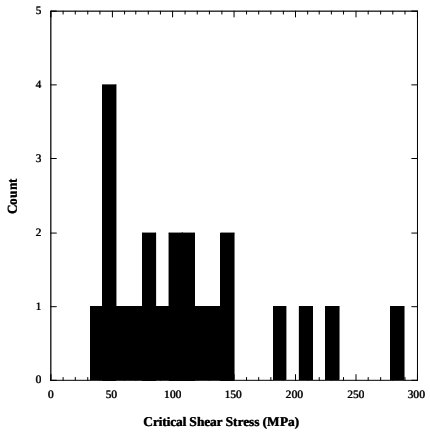

Figure 2. The experimentally determined critical shear stresses for irradiated copper.

Higher pressure helium bubbles result in a different dislocation interaction mechanism. The MD simulations reveal that super-jogs form on the dislocation line, in addition to the shearing of the helium bubble. The super-jogs form as a consequence of the interaction and absorption of the self-interstitial clusters produced by the over-pressurized helium bubbles. Additional details of this mechanism will be presented in future publications.

SUMMARY AND FUTURE WORK

The results presented in this paper demonstrate the use of the latest simulation and experimental techniques to probe the underlying mechanisms governing the mechanical properties of irradiated metals. Reasonable agreement between experiments and simulations are found for the critical shear stress of under pressurized He bubbles in FCC metals. The internal pressure of the bubbles influences the critical shear stress as well as the dislocation interaction and bypass mechanism. Future work will further examine the effect of internal gas pressure, as well as the effect of

dislocation morphology and the geometry on the dislocation/obstacle interactions.

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